

AD-A110 606

WASHINGTON UNIV SEATTLE DEPT OF CHEMISTRY

F/G 7/4

VIBRATIONAL ENERGY TRANSFER AND PYROLYSIS OF NITROMETHANE BY TH--ETC(U)

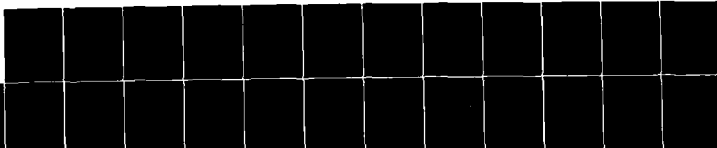
JAN 82 W YUAN, B S RABINOVITCH, R TOSA

N00014-75-C-0690

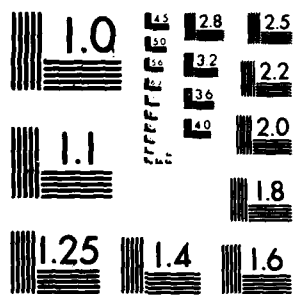
NL

UNCLASSIFIED

1 1 1



END
DATE
FILMED
3 42
DTIC



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A.

LEVEL

12

Vibrational Energy Transfer and Pyrolysis of Nitromethane
by the Variable Encounter Method

by W. Juan, B. S. Rabinovitch and R. Tosa

Department of Chemistry BG-10, University of Washington
Seattle, Washington 98195

Technical Report No. NR092-549-TR24

Contract N00014-75-C-0690, NR-092-549

January 15, 1982

DTIC
ELECTRONIC
FEB 9 1982
S H

Prepared for Publication in
Journal of Physical Chemistry

OFFICE OF NAVAL RESEARCH
Department of the Navy
Code 473
800 N. Quincy
Arlington, VA 22217

Reproduction in whole or in part is permitted for any purpose of
the United States Government. This document has been approved for
public release; its distribution is unlimited.

AD A110606

DTIC FILE COPY

370414

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER NR092-549-TR24	2. GOVT ACCESSION NO. AD-A110606	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Vibrational Energy Transfer and Pyrolysis of Nitromethane by the Variable Encounter Method		5. TYPE OF REPORT & PERIOD COVERED Technical
7. AUTHOR(s) W. Yuan, B. S. Rabinovitch, and R. Tosa		6. PERFORMING ORG. REPORT NUMBER
9. PERFORMING ORGANIZATION NAME AND ADDRESS Professor B. S. Rabinovitch Department of Chemistry BG-10 University of Washington Seattle, WA 98195		8. CONTRACT OR GRANT NUMBER(s) N00014-75-C-0690 NR092-549
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research, Code 473 Department of the Navy 800 N. Quincy Arlington, VA 22217		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		12. REPORT DATE January 15, 1982
		13. NUMBER OF PAGES 20
		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) This document has been approved for public release; its distribution is unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report) Prepared for publication in J. Phys. Chem.		
18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Energy Transfer Surfaces Gases Unimolecular Reaction High Temperature Vibrational Relaxation Nitromethane		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The pyrolysis of nitromethane has been studied by the Variable Encounter Method (VEM) at temperatures from 816 K to 1092 K with two reactors of differing geometry having fused silica surfaces. The probability of reaction per collision with the reactor surface was measured. The down energy transition jump size, $\langle \Delta E' \rangle$, was determined. It decreased with increasing wall temperature. A comparison is made of $\langle \Delta E' \rangle$ with previous results reported to date for other substrate molecules. Nitromethane is one of the more efficient energy transfer agents. However, in addition to the size (vibrational eigenstate density) and the polarity of the molecules, the nature of the hot surface seems also to play a role.		

DD FORM 1 JAN 73 1473

EDITION OF 1 NOV 69 IS OBSOLETE
S/N 0102 LF 014 6601

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

Vibrational Energy Transfer and Pyrolysis of Nitromethane
by the Variable Encounter Method

by W. Yuan,[†] B. S. Rabinovitch and R. Tosa

Department of Chemistry BG-10, University of Washington
Seattle, Washington 98195

Abstract

The pyrolysis of nitromethane has been studied by the Variable Encounter Method (VEM) at temperatures from 816 K to 1092 K with two reactors of differing geometry having fused silica surfaces. The probability of reaction per collision with the reactor surface was measured. The down energy transition jump size, $\langle \Delta E' \rangle$, was determined. It decreased with increasing wall temperature. A comparison is made of $\langle \Delta E' \rangle$ with previous results reported to date for other substrate molecules. Nitromethane is one of the more efficient energy transfer agents. However, in addition to the size (vibrational eigenstate density) and the polarity of the molecules, the nature of the hot surface seems also to play a role.

Accession No.	
NTIS	
AD	
UN	
DTIC	
By	
Distribution	
Available to	
Notes	
1	
A	



Introduction

Nitromethane is a widely investigated species because of its importance in a number of phenomena including the mechanism of gas phase nitration of hydrocarbons, the mechanism of formation of photochemical smog, and the chemistry of propellants. A large amount of work¹⁻⁶ has been devoted to the study of the kinetics and mechanism of the thermal decomposition of nitromethane. However, virtually no attention has been paid to the study of vibrational energy transfer involving this species. Of course, collisional activation and deactivation is a fundamental physical process of great ubiquity. Since nitromethane is a highly polar compound, it is also of interest to study the behavior of this molecule by the VEM method which has been applied recently to a variety of molecules, principally non-polar hydrocarbons.^{7,8} By this technique, vibrational relaxation in the transient region may be studied, in principle, on a collision-by-collision basis.

In this method, a molecule equilibrated at some low temperature in a reservoir flask is allowed to enter a reactor of variable dimensions, say cylindrical, heated to reaction temperature (called an encounter). Two events are possible: the molecule may escape from the finger after a sequence of collisions with the hot wall; or the series of vibrational relaxation collisions with the wall may be terminated by a reaction event. Only subjects for which the decomposition reaction is a homogeneous process have been chosen for study. By varying the geometry of the finger, the average residence time of the molecule in the hot reaction zone can be varied; and the average number m of successive collisions that occur before the molecule exits from the finger (and re-equilibrates with the cold wall) can therefore be varied. The average reaction probability per encounter can be measured experimentally for different fingers, and a suitable

energy transfer model may be estimated by fitting the data. The collision events themselves may be simulated by a Monte Carlo calculation using the known reactor geometry; and a distribution function $f(n,m)$ may be found for the number of sequential collisions n that occur per encounter with a reactor of given m ($m = \bar{n}$).

In this paper we describe the study of nitromethane in two silica reactors at temperatures between 800 K and 1100 K.

Experimental

Nitromethane (Aldrich Chemical Company, 99%, spectrophotometric grade) was used without purification. Gas chromatographic analysis showed that it contained less than 0.5% nitroethane.

As was described previously,⁸ the apparatus consisted of a 1-liter fused quartz spherical reservoir flask which had two quartz cylindrical finger reactors blown on to the surface. These fingers were of cylindrical geometry having length/radius ratios of ~ 1.7 and ~ 6.4 , corresponding to mean numbers of sequential collisions, $m = 5.0$ and 14.4 , respectively. Each finger could be separately heated in a stainless steel furnace block which was maintained by ceramic clamshell Kanthal electric heaters. The temperature of each finger was measured with five chromel-alumel thermocouples cemented separately to the outside of the reactor finger. Typical reactor finger temperatures were ~ 800 K to ~ 1100 K; flask reservoir temperatures were 400 K to 480 K. The temperature variation during the run time was $\pm 1^\circ\text{C}$ and along the finger length was $\pm 10^\circ\text{C}$. The temperature of the reactor was estimated by simple averaging. The effective temperature of the cold flask was suitably weighted by surface area, but calculation showed that the effect on the theoretical calculation due to a change of the flask temperature by as much as 50°K was negligible. Before a run, the reactor and flask reservoir were evacuated to approximately $3 - 5 \times 10^{-6}$ torr. Reaction run pressures were in the range $7 - 8 \times 10^{-4}$ torr. Reaction time varied from several minutes to ten hours, depending on the reaction temperature. The reaction percentage varied between 2% to 40%. At the end of a run, the reaction mixture was expanded from the reactor into a liquid nitrogen trap.

Separation of the reaction products was made at 100°C on a 1-m column of 3-mm copper tubing packed with Porapak Q. The detector was FID. Acetonitrile, which is inert under these conditions,

was used as an internal standard against which the disappearance of substrate could be accurately measured. No attempt was made to monitor all of the product species, which for this system are very numerous.¹⁻⁵

Surface Seasoning

The surface condition of the hot finger had a significant influence on the observed rate constant. If the surface were seasoned with reactant itself as has been customary in all previous work — a technique that has led to minimal and reproducible rates of reaction — the rate constant became progressively higher although eventually leveling off. This suggested the possible presence of surface catalysis. It was found that oxidizing the surface at 1100 K with 30-40 torr pure oxygen for several hours and then evacuating the reactor to $3 - 5 \times 10^{-6}$ torr gave reproducible results and minimal rates of reaction. The oxidation procedure was carried out at each temperature studied.

Results and Discussion

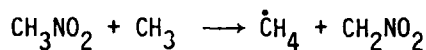
The thermal decomposition reaction obeys the first-order law. This is illustrated in Fig. 1. The apparent rate constants are summarized in Table I. Each tabulation is the average of from three to four determinations from separate runs. As Fig. 2 shows, the Arrhenius relation (which no longer has a simple meaning here) was satisfied for this temperature range. The apparent activation energies calculated from Fig. 2 are $38.8 \text{ kcal mole}^{-1}$, for the $m = 5$ finger, and $42.4 \text{ kcal mole}^{-1}$, for the $m = 14.4$ finger. The latter value, being closer to the low pressure steady state value, should, of course, be the higher one.

There exist several different experimental sets of high-pressure Arrhenius parameters for this reaction.¹⁻⁶ We chose to use the measurement of Glanzer and Troe,⁵ $E_a = 58.5 \text{ kcal mole}^{-1}$, which is quite close to the value calculated by Benson and O'Neal⁶ from thermodynamic quantities and mechanistic considerations. Since this activation energy is the highest of all those reported, we are inclined to believe that this choice is optimal. The GT and BO values for the frequency factor are peculiarly different, but these quantities have no bearing on our results; only E_a enters, i.e., the critical threshold E_0 , since our data were taken in the second-order region.

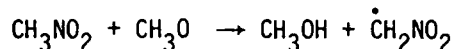
The vibrational spectrum of nitromethane has been assigned⁹ (see App. I). The value of E_0 for nitromethane was calculated to be $54.4 \text{ kcal mole}^{-1}$, with use of the average temperature 1150 K over the range used by GT and the activated complex model of App I.

The average probability of decomposition per collision with the hot wall in a reactor of given m -value, $\bar{P}_c(m)$, was calculated from the apparent first-order rate constants, the known reactor dimensions and the reservoir flask temperature. Since our rates were calculated from nitromethane disappearance, it is necessary to consider the possible extent of chain or sensitized character

of nitromethane pyrolysis. According to Perche's¹⁰ simplified mechanism used for computer simulation kinetics, the important secondary radical reactions which cause significant decomposition of nitromethane are



and



From the detailed product construction given by these authors at 700 K, the additional decomposition fraction of the parent is estimated at approximately 30%. Since these free radical reactions have low critical thresholds, the temperature increase in our system to the range 800 K-1000 K favors the unimolecular decomposition relative to these abstraction processes. Moreover, in our system the total pressure is very much lower than in the usual pyrolytic conditions so that it is expected that the importance of second order reactions are even further reduced. In fact, our rate constants were unaltered within experimental error when the reaction pressure was increased from 3×10^{-4} torr to 3×10^{-3} torr. This implies that in our system the observed rate constant is virtually independent of the role played by bimolecular secondary reactions and we have adopted the observed rate values as the correct ones. The $\bar{P}_c(m)$ values are collected in Table II and Fig. 3 for $m = 5$ and 14.4.

The computer simulation of the encounter activation process has been described elsewhere.^{7,15} Two models have been used to characterize the probability, p_{ij} of a down energy transition, ΔE , by the molecule from energy E_j to energy E_i :

Model FG (flat gaussian, i.e., ΔE_{mp} independent of E_j),

$$p_{ij} = A_1 \exp(-(\Delta E - \Delta E_{mp})^2 / 2\sigma^2) ;$$

Model BE (exponentially weighted Boltzmann),

$$p_{ij} = A_2 N(E_i) \exp(E_i/RT) \exp(-\Delta E / \langle \Delta E \rangle) .$$

The correlation table used in the computer simulation is given in Table III.

The correlation coefficient C_j is defined as the probability that molecules which have already experienced j collisions with the hot wall will have at least the $(j+1)$ th collision, i.e., $C_j = \frac{\sum_{i=j+1}^{\infty} n_i}{\sum_{i=j}^{\infty} n_i}$, where n_i is the sum of the molecules in the distribution vector left after i collisions. The correlation coefficients summarize the varying probability of a molecule remaining in the reactor after each wall collision. The parameters of each particular model distribution were adjusted to provide theoretical agreement with the experimental curve for the $m = 5$ finger; the parameters so chosen were then used to calculate a theoretical curve for the $m = 14.4$ finger.

Fit is made to the $m = 5$ curve because it provides greater sensitivity to model detail than does the $m = 14.4$ curve which lies closer to the steady state value. The graphs are shown in Fig. 3. It can be seen that the theoretical curves are close to the experimental value for $m = 14.4$, showing good concordance between the two sets of experimental data. The BE model fits the data somewhat better than the FG model but there is little to choose between them. A set of parameters for the FG model that exactly fit the experimental $m = 14.4$ data may be calculated and give somewhat higher values of $\langle \Delta E' \rangle$.

Calculated steady state curves ($m = \infty$) as well as the strong collider curve are also given in Fig. 3, and it appears that the hot wall will approach the strong collider behavior when the temperature falls substantially below 800 K. Once again, the trend observed in previous VEM studies¹¹⁻¹³ of increasing strength of collisions with decreasing temperature is borne out. (However, the lowest temperature value for $m = 14.4$ appears somewhat too high.) The effective average energy of down transitions, $\langle \Delta E' \rangle$ for models BE and FG together with their parameters are summarized in Table IV.

Comparison with the previous results by the VEM method is made in Table V. A rough rule that the down jump energy transfer efficiency per collision of the substrate, declines with increasing size (i.e., increasing vibrational eigenstate density) of the molecule seemed evident from earlier studies with various hydrocarbon reactants.⁸ Also, it was shown that the polar molecule, iodopropane ($\mu = 2.0$ D), seems more efficient in energy transfer than non-polar ones, due to the longer sticking time that gives rise to more complete accommodation. The measured efficiency for highly polar nitromethane ($\mu = 3.6$ D), while one of the more efficient in Table IV, seems a little lower than expected (which, incidentally, also belies any significant role for surface catalysis). However, we note that in the present work an oxidized surface was used instead of the surface seasoned by the reactant itself, as in our previous studies, so that we may be seeing an effect of different energy transfer efficiency of the surface. Indeed, as mentioned above under Experimental, the rate (not reported) on a seasoned surface was larger; calculated values of the energy transfer on such a surface were found and gave magnitudes that even exceed those for iodopropane.

Clearly, apart from the polarity or size of molecules, the nature of the surface must play a significant role in molecule-surface relaxation process. We will attempt to clarify this feature in future studies.

Acknowledgment

We thank the Office of Naval Research for their support of this work.

Table I. Apparent Rate Constants for Decomposition

<u>m</u>	<u>T(K)</u>	<u>$10^6 k \text{ (sec}^{-1}\text{)}$</u>	
5.0	870	4.1	
		5.1	Av. 4.5 ± 0.6^a
		4.2	
	987	59	
		70	Av. 69 ± 8
		64	
		84	
	1069	290	
		290	Av. 305 ± 12
		320	
		320	
14.4	816	12.5	
		10.1	Av. 10.8 ± 1.4
		8.4	
		12.2	
	907	139	
		143	Av. 148 ± 14
		176	
		133	
	1013	2000	
		1760	Av. 1750 ± 100
		1780	
		1470	
	1092	8200	
		8000	Av. 8000 ± 200
		7800	

a) Standard deviation of the mean

Table II. Experimental values of $\bar{P}_c(m)$

<u>m</u>	<u>T(K)</u>	<u>$10^8 \bar{P}_c(m)$</u>
5.0	870	1.3
	987	20
	1069	87
14.4	816	1.2
	907	16
	1013	180
	1092	800

Table III. Correlation Coefficients C_n

<u>n/m</u>	<u>5</u>	<u>14.4</u>
1	0.750	0.759
2	0.788	0.833
3	0.800	0.889
4	0.809	0.907
5	0.815	0.921
6	0.819	0.930
7	0.822	0.937
8	0.824	0.942
9	0.824	0.946
10		0.950
11		0.952
12		0.954
13		0.956
14		0.957
15		0.958
16		0.958
17		
18		

Table IV. Energy Transfer Parameters for Nitromethane

	<u>T(K)</u>	<u>816</u>	<u>907</u>	<u>1013</u>	<u>1092</u>
FG	$\langle \Delta E_{mp} \rangle$	2440	1960	1760	1700
	$\langle \Delta E' \rangle$	2700	2170	1950	1880
BE	$\langle \Delta E \rangle$	911	943	981	1090
	$\langle \Delta E' \rangle_{E_0}^a$	4970	4100	3360	3355

a) Energy level dependent value; given here at $E = E_0$

Table V. Comparison of $\langle \Delta E' \rangle$ (cm^{-1}) for Different Molecules

Molecule	$E_o/(\text{kcal mole}^{-1})$	n_t^a	Model	$\langle \Delta E' \rangle \text{ (cm}^{-1}\text{)}^b$					Ref.
				800 K	900 K	1000 K	1100 K		
Nitromethane	54.4	15	G	2840	2200	1960	1880	this work	
1-Iodopropane	48.5	27	G	3015				11	
Cyclopropane	64	21	G	3050	2400	2100	2000	8	
				3200	2500	2170	2040	14	
Cyclopropane-d ₆	65.5	21	G	2300	2040	1890	1860	8	
Cyclobutene	33	24	G	2010				15	
Cyclobutane	63	30	Exp ^c	2180	1800	1600	1480	16	
			G	2700	2125	1925	1875		
Methylcyclopropane	61	30	Exp	1860	1550	1440	1415	17	

a) The number of internal degrees of freedom

b) Some values obtained by interpolation or extrapolation

c) Flat exponential model

Appendix

Vibrational frequencies and parameters for RRKM calculations (cm^{-1})

Nitromethane molecule:

3048(2), 2965, 1582, 1488, 1449, 1413, 1384, 1153, 1097, 921, 647, 599,
476, internal rotation ($\sigma = 6$).

Activated complex:

3048(2), 2965, 1582, 1488, 1449, 1413, 1384, 647, 200(2), 120(2), internal
rotation ($\sigma = 6$).

$E_0 = 54.4 \text{ kcal mole}^{-1}$

$F = 1.3$

References

- [†] Visiting Scholar; permanent address: Department of Chemistry and Chemical Engineering, Qinghua University, Beijing, China.
1. Dubikhin, V. V.; Nazin, G. M.; Manelis, G. B. Akademiia Nauk SSSR, Chemical Science Div. Bull. 1971, 1247.
 2. Crawforth, C. G.; Waddington, D. J. J. Phys. Chem. 1970, 74, 2793; Trans. Faraday Soc. 1969, 65, 1334.
 3. Nazin, G. M.; Manelis, G. B.; Dubovitskii, F. I. Russian Chemical Reviews 1963, 37, 603.
 4. Zaslanko, I. S.; Kogarko, S. M.; Mozhukhin, E. B.; Petrov, Yu. P. Kinetics and Catalysis 1972, 13, 1001
 5. Glanzer, K.; Troe, J. Helv. Chim. Acta 1972, 55, 2884; Troe, J. J. Chem. Phys. 1977, 66, 4758.
 6. Benson, S. W.; O'Neal, H. E. "Kinetic Data on Gas Phase Unimolecular Reactions" NSRDS, Nat. Bur. Stds. #21, 1970, p. 473.
 7. Kelley, D. F.; Zalotai, L.; Rabinovitch, B. S. Chem. Phys. 1980, 46, 379.
 8. Yuan, W.; Tosa, R.; Chao, K.-J.; Rabinovitch, B. S. Chem. Phys. Lett. in press.
 9. Wells, A. J.; Wilson, Jr., E. B. J. Chem. Phys. 1941, 9, 314.
 10. Perche, A.; Tricot, J. C.; Lucquin, M. J. Chem. Research(S) 1979, 116, 1979, 304; 1979, 306.
 11. Wolters, F. C.; Chao, K.-J.; Rabinovitch, B. S. Int. J. Chem. Kin. 1982, in press.
 12. Kasai, T.; Kelley, D. F.; Rabinovitch, B. S. Chem. Phys. Lett. 1981, 81, 126.
 13. Arakawa, R.; Kelley, D. F.; Rabinovitch, B. S. J. Chem. Phys. 1981,
 14. Flowers, M. C.; Wolters, F. C.; Kelley, D. F.; Rabinovitch, B. S. J. Phys. Chem. 1981, 85, 849.
 15. Wolters, F. C.; Flowers, M. C.; Rabinovitch, B. S. J. Phys. Chem. 1981, 85, 589.
 16. Flowers, M. C.; Wolters, F. C.; Barton, B. D.; Rabinovitch, B. S. Chem. Phys. 1980, 47, 189.
 17. Kelley, D. F.; Kasai, T.; Rabinovitch, B. S. J. Chem. Phys. 1980, 73, 5611.

Figure Captions

Fig. 1 First order law plots of $\ln(a-x)$ versus ct (sec)

□ , $T = 870$ K, $c = 10^{-5}$; $\triangle = T = 1068$ K, $c = 10^{-2}$

Fig. 2 Arrhenius plots of $\log_{10} k$ vs $1/T$ for the $m = 5.0$ and $m = 14.4$ reactors.

Fig. 3 Plots of $\bar{P}_c(m)$ versus $T(K)$ for the $m = 5.0$ and $m = 14.4$ reactors.

■ are the experimental points for the $m = 5.0$ reactor;

□ are the experimental points for the $m = 14.4$ reactor;

— and - - - - are theoretical plots of BE model and FG model, fitted at $m = 5.0$, for the $m = 14.4$ reactor. The theoretical curve for the strong collider (SC) and for the $m = \infty$, steady-state case, calculated with the $m = 5.0$ parameters of the BE model, are also shown.

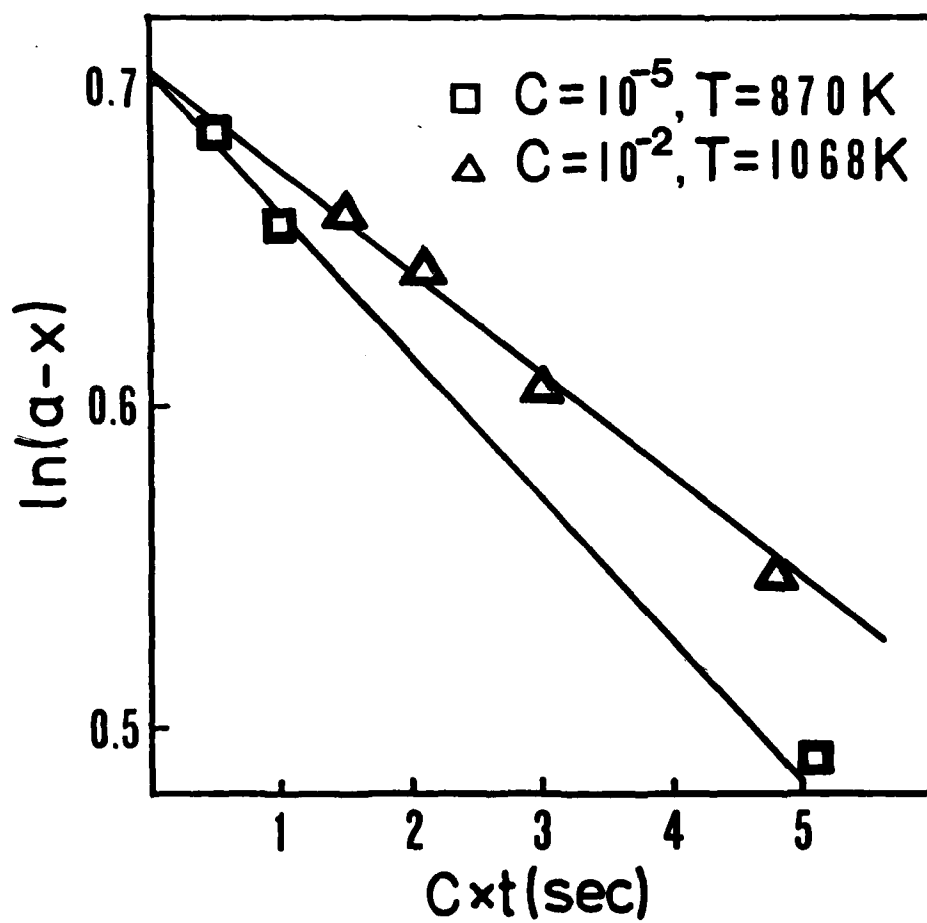


Fig. 1. *Yuan et al.*

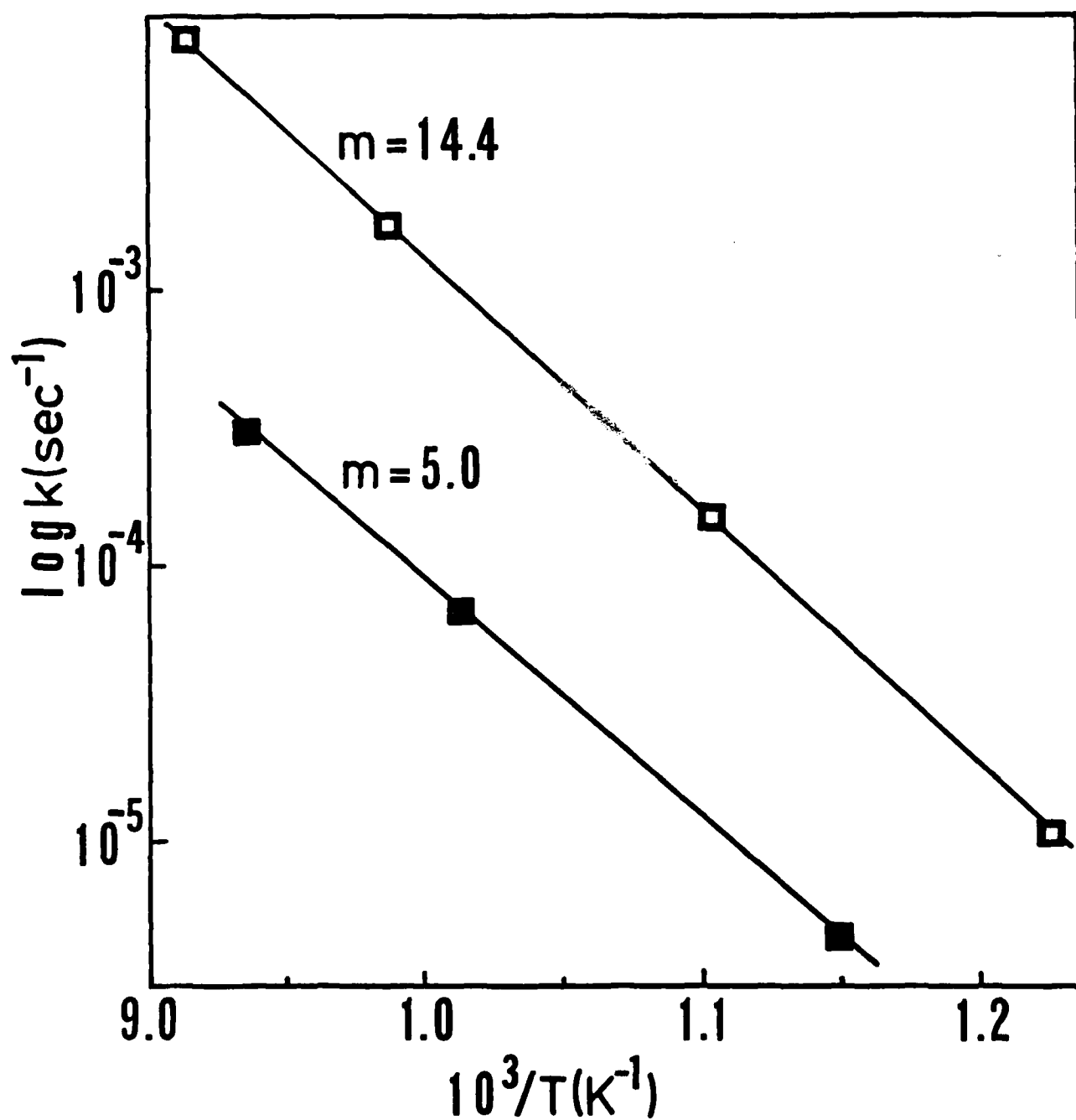


Fig. 2. Huan et al.

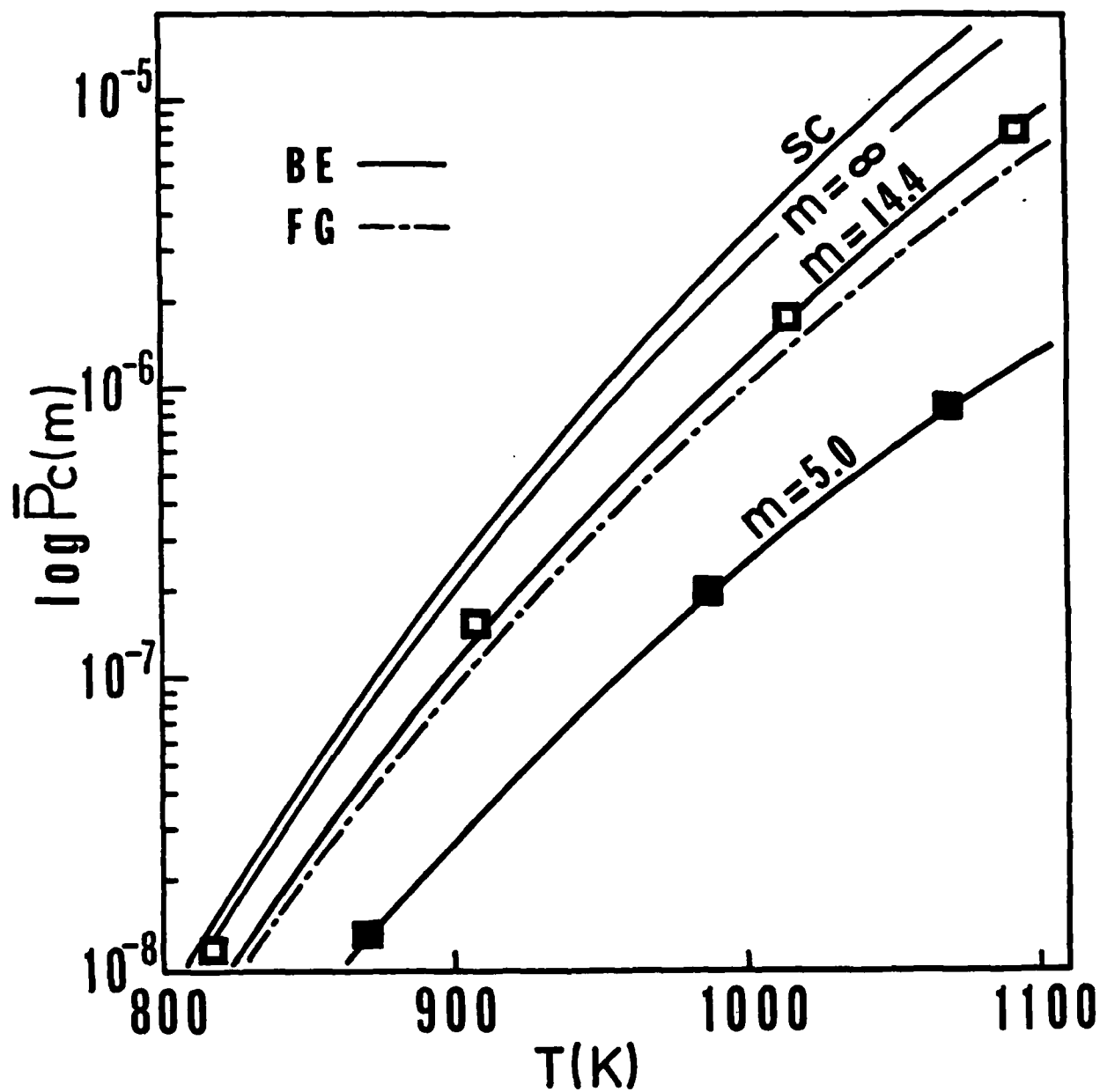


Fig 3 Uzun et al

INIT

DISTRIBUTION LIST

January 15, 1982

	<u>No. Copies</u>		<u>No. Copies</u>
Dr. L.V. Schmidt Assistant Secretary of the Navy (R,E, and S) Room 5E 731 Pentagon Washington, D.C. 20350	1	Dr. F. Roberto Code AFRPL MKPA Edwards AFB, CA 93523	1
Dr. A.L. Slafkosky Scientific Advisor Commandant of the Marine Corps Code RD-1 Washington, D.C. 20380		Dr. L.H. Caveny Air Force Office of Scientific Research Directorate of Aerospace Sciences Bolling Air Force Base Washington, D.C. 20332	1
Dr. Richard S. Miller Office of Naval Research Code 413 Arlington, VA 22217	10	Mr. Donald L. Ball Air Force Office of Scientific Research Directorate of Chemical Sciences Bolling Air Force Base Washington, D.C. 20332	1
Mr. David Siegel Office of Naval Research Code 260 Arlington, VA 22217	1	Dr. John S. Wilkes, Jr. FJSRL/NC USAF Academy, CO 80840	1
Dr. R.J. Marcus Office of Naval Research Western Office 1030 East Green Street Pasadena, CA 91106	1	Dr. R.L. Lou Aerojet Strategic Propulsion Co. P.O. Box 15699C Sacramento, CA 95813	1
Dr. Larry Peebles Office of Naval Research East Central Regional Office 666 Summer Street, Bldg. 114-D Boston, MA 02210	1	Dr. V.J. Keenan Anal-Syn Lab Inc. P.O. Box 547 Paoli, PA 19301	1
Dr. Phillip A. Miller Office of Naval Research San Francisco Area Office One Hallidie Plaza, Suite 601 San Francisco, CA 94102	1	Dr. Philip Howe Army Ballistic Research Labs ARRADCOM Code DRDAR-BLT Aberdeen Proving Ground, MD 21005	1
Mr. Otto K. Heiney AFATL - DLDL Eglin AFB, FL 32542	1	Mr. L.A. Watermeier Army Ballistic Research Labs ARRADCOM Code DRDAR-BLI Aberdeen Proving Ground, MD 21005	1
Mr. R. Geisler ATTN: MKP/MS24 AFRPL Edwards AFB, CA 93523	1	Dr. W.W. Wharton Attn: DRSMI-RKL Commander U.S. Army Missile Command Redstone Arsenal, AL 35898	1

6/81

INIT

DISTRIBUTION LIST

	<u>No. Copies</u>		<u>No. Copies</u>
Mr. J. Murrin	1	Dr. A. Nielsen	1
Naval Sea Systems Command		Naval Weapons Center	
Code 62R2		Code 385	
Washington, D.C. 20362		China Lake, CA 93555	
Dr. P.J. Pastine	1	Dr. R. Reed, Jr.	1
Naval Surface Weapons Center		Naval Weapons Center	
Code R04		Code 388	
White Oak		China Lake, CA 93555	
Silver Spring, MD 20910			
Mr. L. Roslund	1	Dr. L. Smith	1
Naval Surface Weapons Center		Naval Weapons Center	
Code R122		Code 3205	
White Oak		China Lake, CA 93555	
Silver Spring, MD 20910			
Mr. M. Stosz	1	Dr. B. Douda	1
Naval Surface Weapons Center		Naval Weapons Support Center	
Code R121		Code 5042	
White Oak		Crane, IN 47522	
Silver Spring, MD 20910			
Dr. E. Zimmet	1	Dr. A. Faulstich	1
Naval Surface Weapons Center		Chief of Naval Technology	
Code R13		MAT Code 0716	
White Oak		Washington, D.C. 20360	
Silver Spring, MD 20910			
Dr. D.R. Derr	1	LCDR J. Walker	1
Naval Weapons Center		Chief of Naval Material	
Code 388		Office of Naval Technology	
China Lake, CA 93555		MAT, Code 0712	
		Washington, D.C. 20360	
Mr. Lee N. Gilbert	1	Mr. Joe McCartney	1
Naval Weapons Center		Naval Ocean Systems Center	
Code 3205		San Diego, CA 92152	
China Lake, CA 93555			
Dr. E. Martin	1	Dr. S. Yamamoto	1
Naval Weapons Center		Marine Sciences Division	
Code 3858		Naval Ocean Systems Center	
China Lake, CA 93555		San Diego, CA 91232	
Mr. R. McCarten	1	Dr. G. Bosmajian	1
Naval Weapons Center		Applied Chemistry Division	
Code 3272		Naval Ship Research & Development	
China Lake, CA 93555		Center	
		Annapolis, MD 21401	
		Dr. H. Shuey	1
		Rohm and Haas Company	
		Huntsville, AL 35801	

INIT

DISTRIBUTION LIST

	<u>No. Copies</u>		<u>No. Copies</u>
Mr. R. Brown	1	Dr. J. Schnur	1
Naval Air Systems Command		Naval Research Lab.	
Code 330		Code 6510	
Washington, D.C. 20361		Washington, D.C. 20375	
Dr. H. Rosenwasser	1	Mr. R. Beauregard	1
Naval Air Systems Command		Naval Sea Systems Command	
AIR-310C		SEA 64E	
Washington, D.C. 20360		Washington, D.C. 20362	
Mr. B. Sobers	1	Mr. G. Edwards	1
Naval Air Systems Command		Naval Sea Systems Command	
Code 03P25		Code 62R3	
Washington, D.C. 20360		Washington, D.C. 20362	
Dr. L.R. Rothstein	1	Mr. John Boyle	1
Assistant Director		Materials Branch	
Naval Explosives Dev.		Naval Ship Engineering Center	
Engineering Dept.		Philadelphia, PA 19112	
Naval Weapons Station			
Yorktown, VA 23691		Dr. H.G. Adolph	1
Dr. Lionel Dickinson	1	Naval Surface Weapons Center	
Naval Explosive Ordnance		Code R11	
Disposal Tech. Center		White Oak	
Code D		Silver Spring, MD 20910	
Indian Head, MD 20640		Dr. T.D. Austin	1
Mr. C.L. Adams	1	Naval Surface Weapons Center	
Naval Ordnance Station		Code R16	
Code PM4		Indian Head, MD 20640	
Indian Head, MD 20640		Dr. T. Hall	1
Mr. S. Mitchell	1	Code R-11	
Naval Ordnance Station		Naval Surface Weapons Center	
Code 5253		White Oak Laboratory	
Indian Head, MD 20640		Silver Spring, MD 20910	
Dr. William Tolles	1	Mr. G.L. Mackenzie	1
Dean of Research		Naval Surface Weapons Center	
Naval Postgraduate School		Code R101	
Monterey, CA 93940		Indian Head, MD 20640	
Naval Research Lab.	1	Dr. K.F. Mueller	1
Code 6100		Naval Surface Weapons Center	
Washington, D.C. 20375		Code R17	
		White Oak	
		Silver Spring, MD 20910	

DISTRIBUTION LIST

	<u>No. Copies</u>		<u>No. Copies</u>
Dr. R.G. Rhoades Commander Army Missile Command DRSMI-R Redstone Arsenal, AL 35898	1	Dr. E.H. Debutts Hercules Inc. Baccus Works P.O. Box 98 Magna, UT 84044	1
Dr. W.D. Stephens Atlantic Research Corp. Pine Ridge Plant 7511 Wellington Rd. Gainesville, VA 22065	1	Dr. James H. Thacher Hercules Inc. Magna Baccus Works P.O. Box 98 Magna, UT 84044	1
Dr. A.W. Barrows Ballistic Research Laboratory USA ARRADCOM DRDAR-BLP Aberdeen Proving Ground, MD 21005	1	Mr. Theodore M. Gilliland Johns Hopkins University APL Chemical Propulsion Info. Agency Johns Hopkins Road Laurel, MD 20810	1
Dr. C.M. Frey Chemical Systems Division P.O. Box 358 Sunnyvale, CA 94086	1	Dr. R. McGuire Lawrence Livermore Laboratory University of California Code L-324 Livermore, CA 94550	1
Professor F. Rodriguez Cornell University School of Chemical Engineering Olin Hall Ithaca, NY 14853	1	Dr. Jack Linsk Lockheed Missiles & Space Co. P.O. Box 504 Code Org. 83-10, Bldg. 154 Sunnyvale, CA 94088	1
Defense Technical Information Center DTIC-DDA-2 Cameron Station Alexandria, VA 22314	12	Dr. B.G. Craig Los Alamos National Lab P.O. Box 1663 NSP/DOD, MS-245 Los Alamos, NM 87545	1
Dr. Rocco C. Musso Hercules Aerospace Division Hercules Incorporated Alleghany Ballistic Lab P.O. Box 210 Washington, DC 21502	1	Dr. R.L. Rabie WX-2, MS-952 Los Alamos National Lab. P.O. Box 1663 Los Alamos, NM 87545	1
Dr. Ronald L. Simmons Hercules Inc. Eglin AFATL/DL DL Eglin AFB, FL 32542	1	Dr. R. Rogers Los Alamos Scientific Lab. WX-2 P.O. Box 1663 Los Alamos, NM 87545	1

6/81

DISTRIBUTION LIST

<u>No. Copies</u>	<u>No. Copies</u>
Dr. J.F. Kincaid 1 Strategic Systems Project Office Department of the Navy Room 901 Washington, D.C. 20376	Dr. C.W. Vriesen 1 Thiokol Elkton Division P.O. Box 241 Elkton, MD 21921
Strategic Systems Project Office 1 Propulsion Unit Code SP2731 Department of the Navy Washington, D.C. 20376	Dr. J.C. Hinshaw 1 Thiokol Wasatch Division P.O. Box 524 Brigham City, UT 83402
Mr. E.L. Throckmorton 1 Strategic Systems Project Office Department of the Navy Room 1048 Washington, D.C. 20376	U.S. Army Research Office 1 Chemical & Biological Sciences Division P.O. Box 12211 Research Triangle Park, NC 27709
Dr. D.A. Flanigan 1 Thiokol Huntsville Division Huntsville, AL 35807	Dr. R.F. Walker 1 USA ARRADCOM DRDAR-LCE Dover, NJ 07801
Mr. G.F. Mangum 1 Thiokol Corporation Huntsville Division Huntsville, AL 35807	Dr. T. Sinden 1 Munitions Directorate Propellants and Explosives Defense Equipment Staff British Embassy 3100 Massachusetts Ave. Washington, D.C. 20008
Mr. E.S. Sutton 1 Thiokol Corporation Elkton Division P.O. Box 241 Elkton, MD 21921	Mr. J.M. Frankle 1 Army Ballistic Research Labs ARRADCOM Code DRDAR-BLI Aberdeen Proving Ground, MD 21005
Dr. G. Thompson 1 Thiokol Wasatch Division MS 240 P.O. Box 524 Brigham City, UT 84302	Dr. Ingo W. May 1 Army Ballistic Research Lab ARRADCOM Code DRDAR-BLI Aberdeen Proving Ground, MD 21005
Dr. T.F. Davidson 1 Technical Director Thiokol Corporation Government Systems Group P.O. Box 9258 Ogden, UT 84409	

INIT

6/81

DISTRIBUTION LIST

	<u>No. Copies</u>		
E. J. Palm	1	Dr. Kenneth O Hartman	1
Commander		Hercules Aerospace Division	
Army Missile Command		Hercules Incorporated	
DRSMI-RK		Allegany Ballistics Lab	
Redstone Arsenal, AL 35898		P.O. Box 210	
		Cumberland, MD 21502	
Dr. Merrill K. King	1	Dr. Joyce J. Kaufman	1
Atlantic Research Corp.		The Johns Hopkins University	
5390 Cherokee Avenue		Department of Chemistry	
Alexandria, VA 22314		Baltimore, MD 21218	
Dr. R.J. Bartlett	1	Dr. John K. Dienes	1
Batelle Columbus Laboratories		T-3, MS-216	
505 King Avenue		Los Alamos National Lab	
Columbus, OH 43201		P.O. Box 1663	
Dr. P. Rentzepis	1	Los Alamos, NM 87544	
Bell Laboratories		Dr. H.P. Marshall	1
Murray Hill, NJ 07971		Dept. 52-35, Bldg. 204.2	
Professor Y.T. Lee	1	Lockheed Missile & Space Co.	
Department of Chemistry		3251 Hanover Street	
University of California		Palo Alto, CA 94304	
Berkeley, CA 94720		Professor John Deutsch	1
Professor M. Nicol	1	MIT	
Department of Chemistry		Department of Chemistry	
405 Hilgard Avenue		Cambridge, MA 02139	
University of California		Professor Barry Kunz	1
Los Angeles, CA 90024		College of Sciences & Arts	
Professor S.S. Penner	1	Department of Physics	
University of California		Michigan Technological Univ.	
Energy Center		Houghton, MI 49931	
Mail Code B-010		Dr. R. Bernecker	1
La Jolla, CA 92093		Code R13	
Professor Curt Wittig	1	Naval Surface Weapons Center	
University of Southern CA		White Oak	
Dept. of Electrical Engineering		Silver Spring, MD 20910	
University Park		Dr. C.S. Coffey	1
Los Angeles, CA 90007		Naval Surface Weapons Center	
		Code R13	
		White Oak	
		Silver Spring, MD 20910	

INIT

6/81

DISTRIBUTION LISTNo. Copies

Dr. W. L. Elban Code R13 Naval Surface Weapons Center White Oak Silver Spring, MD 20910	1
Mr. K.J. Graham Naval Weapons Center Code 3835 China Lake, CA 93555	1
Dr. B. Junker Office of Naval Research Code 421 Arlington, VA 22217	1
Prof. H.A. Rabitz Department of Chemistry Princeton University Princeton, NH 08540	1
Dr. M. Farber Space Sciences, Inc. 135 West Maple Avenue Monrovia, CA 91016	1
Mr. M. Hill SRI International 333 Ravenswood Avenue Menlo Park, CA 94025	1
U.S. Army Research Office Engineering Division Box 12211 Research Triangle Park, NC 27709	1
U.S. Army Research Office Metallurgy & Materials Sci. Div. Box 12211 Research Triangle Park, NC 27709	1
Professor G.D. Duvall Washington State University Department of Physics Pullman, WA 99163	1

END

DATE
FILMED

3-82

DTIC